Non-equilibrium chemistry models and directly imaged exoplanets with JWST/MIRI

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Coming soon: In Baudino et al. 2016 (in prep.) we compare 3 models of atmopshere (ATMO, Exo-REM, petitCODE) and 2 models of chemistry (Venot et al. 2012 and Zahnle and Marley 2014)

JWST:
In October 2018 the JWST will be launched with four instruments on board; three instruments, will be operating in the 0.6-5 microns range: NIRISS , NIRCam, NIRSpec,
and one in the 5-28 microns range: MIRI.

MIRI:
coronagraphy,
imaging and spectroscopy

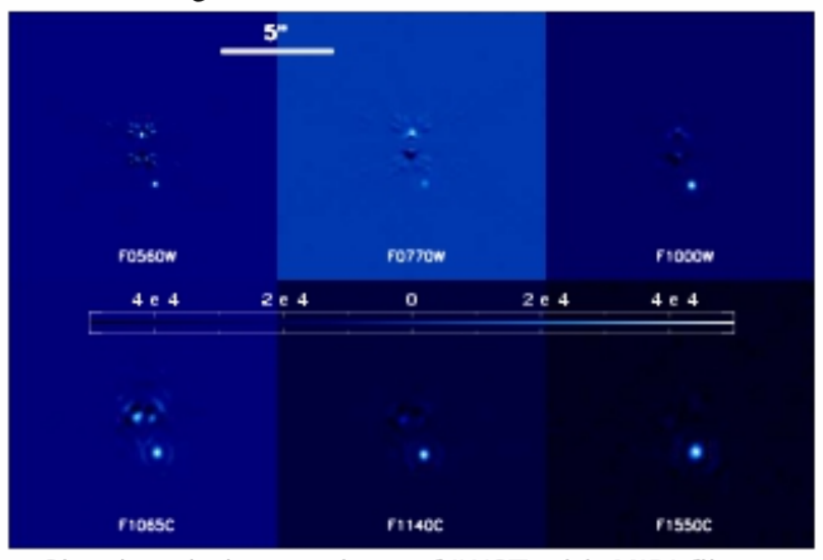
3x four Quadrants Phase Mask (4QPM)
(2 for NH_3)

mid and low spectral resolution

Goal: How JWST (especially MIRI) can help to characterize atmosphere in term of non-equilibrium chemistry ?

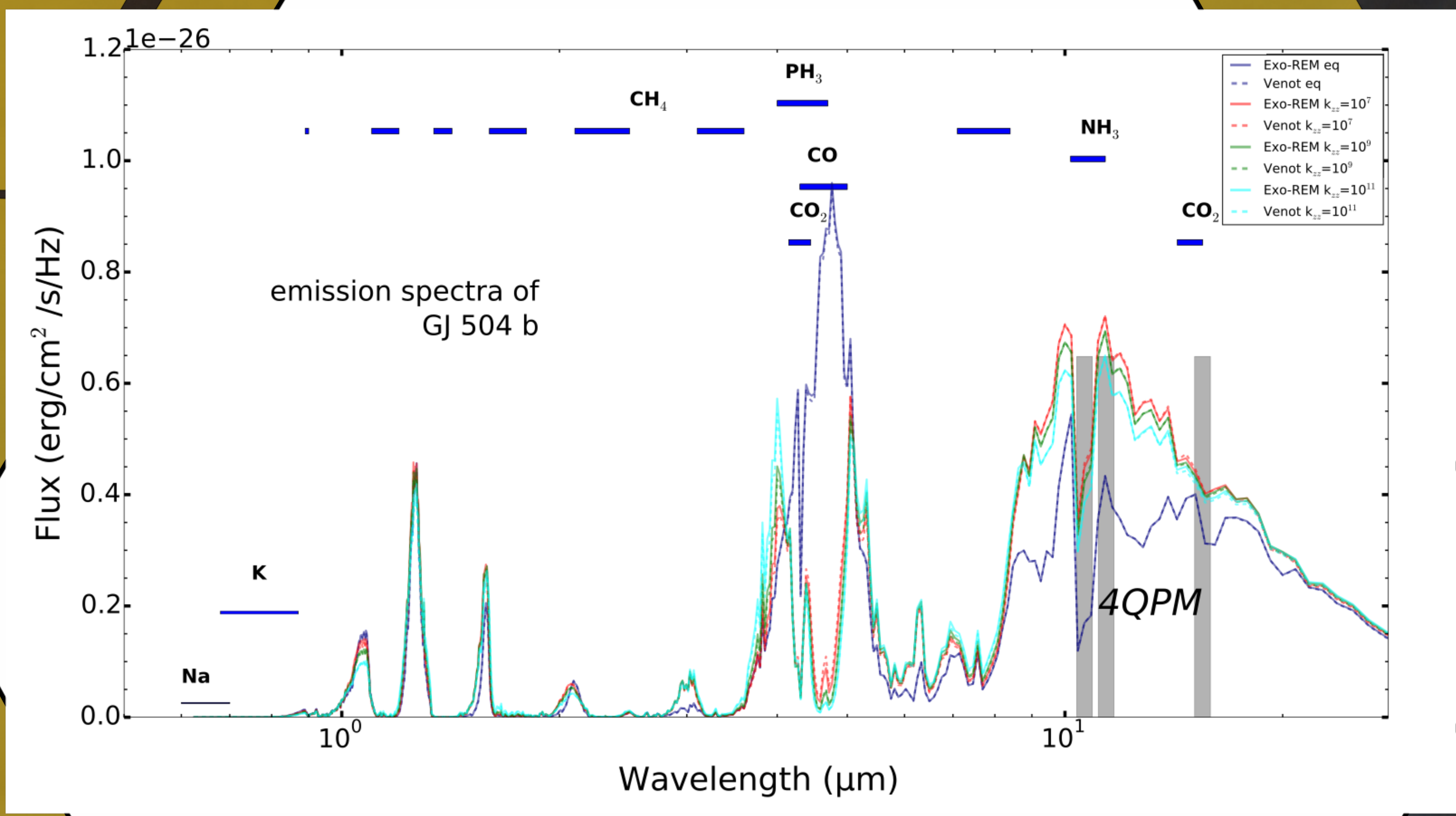
Process: same input temperature profile computed by Exo-REM (without clouds) for two sets of characteristic corresponding to potential targets at chemical equilibrium and for a strong Eddy coefficient K_{zz}, defining non-equilibrium chemistry with two chemical networks (Venot et al. 2012 and Exo-REM adapted form Zahnle and Marley 2014)

Targets:
self-luminous planets (young and hot) faraway from the host star



Simulated observations of JWST with MIRI filters Boccaletti et al. 2015

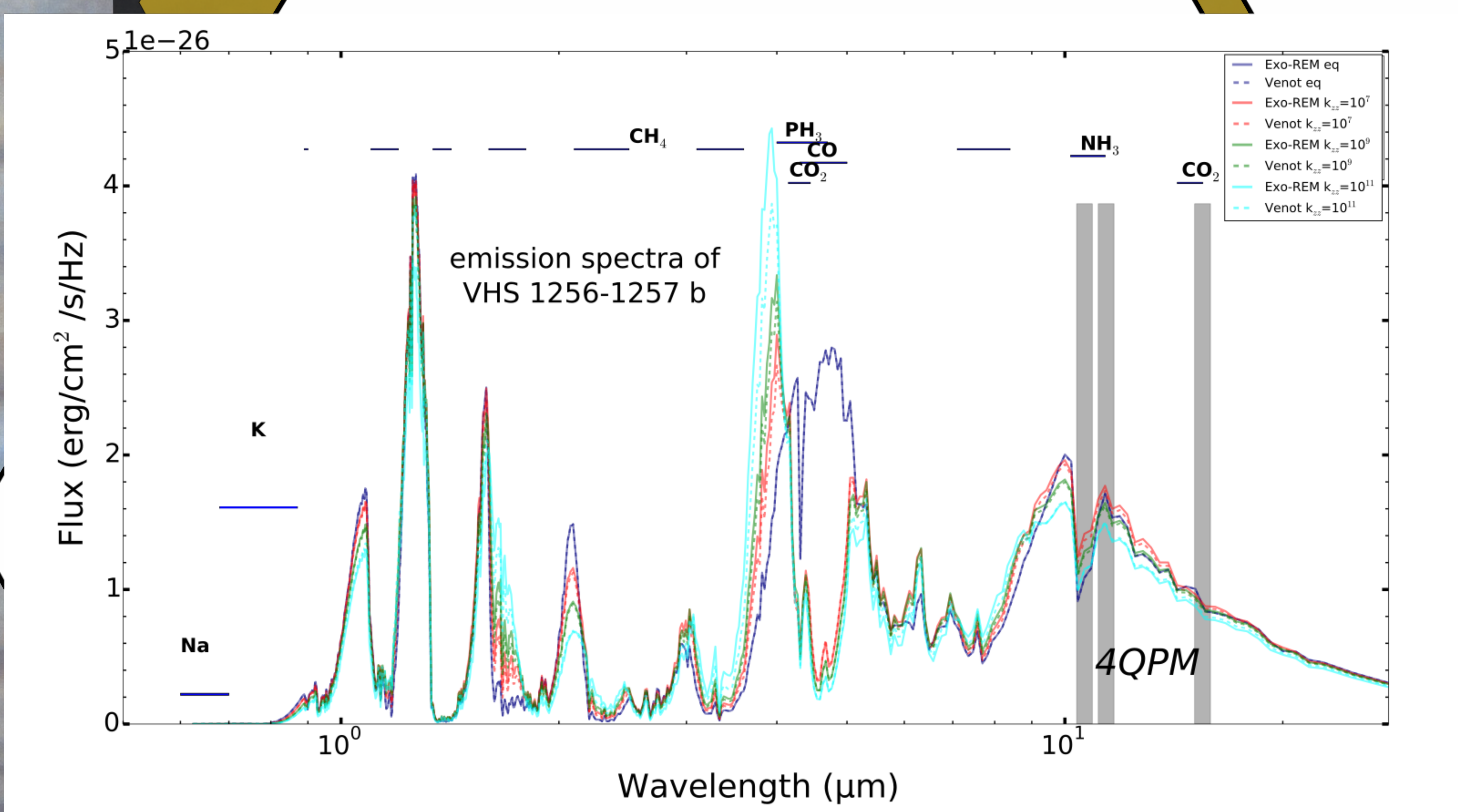
GJ 504 b:
Teff=510 K, log(g)=3.9,
z=0.28 dex



Non-equilibrium chemistry, as expected, is more effective at low temperature (top: GJ 504b, Teff=510 K compared to bottom: VHS 1256-1257 b 880 K).
NH_3, CH_4, CO_2 are molecules with features in MIRI wavelength. The two first are easily observable in both cases. NH_3 depth after 10 μm could allow us to distinguish between equilibrium and non-equilibrium chemistry at low temperature.

Spectroscopic modes of MIRI could also give contains on the Eddy coefficient K_{zz} (parameter defining the non-equilibrium chemistry). 9-10 and 12-15 μm seems good wavelength range to focus-on.

VHS 1256-1257 b
Teff=880 K, log(g)=4.24,
z=0.21 dex



Spectroscopic observations in wavelength between 4 and 5 μm (NIRSpec) seems also to be crucial to study non-equilibrium chemistry because of absorption of the PH_3, CO and CO_2.
This location of spectrum can be useful without high resolution or high signal-to-noise ratio.

Note: PH_3 is an important specie in non-equilibrium chemistry condition, for example in Jupiter, but it is not detected in the spectrum of the coldest known brown dwarf (Skemer et al. 2016 submitted to ApJL).

Non-equilibrium chemistry ?
Non-equilibrium chemistry can strongly affect the composition at observable levels of relatively cold atmospheres, originates from vertical transport from deep hot layers where chemical equilibrium is achieved. When the dynamical timescale (trigged by Eddy coefficient K_{zz}) is shorter than the chemical timescale we observe a freezing of the abundance of some species.

Uncertainties on the chemical network:
Exo-REM takes into account some condensation when Venot et al. 2012 don't (we decided to apply a modification of the initial elemental abundances used in Venot model, corresponding to a sequestration of ~20% of the amount of oxygen in silicate).We observe other differences, without identifying the origin, such as more methane and less water up to 1 bar in Venot et al. 2012, but without strong impact in spectra.

Conclusions:
- JWST will allow us to explore some physical condition of young giant exoplanet such as the non-equilibrium chemistry effect.
- In the MIR CH_4, CO_2 and NH_3 impact spectra and will give constrains to discriminate those effects.
- 4QPM will give constains on abundances of the NH_3, for the major part of already known direct imaged exoplanets.

- NIRSpec observation will be useful to discriminate equilibrium/non-equilibrium.

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Background picture credit: JPL/NASA Voyager 1